Dibromomethane

74-95-3 | DTXSID4021557

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 41.1 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.69e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

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Methanethiol
Measured: 44.4
Predicted: 863

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Vinyl fluoride

Measured: 136

Predicted: 10300

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Epichlorohydrin Measured: 11.2 Predicted: 29.9

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2-Chloroethanol Measured: 43.1 Predicted: 6.87